Archives available at journals.mriindia.com

International Journal on Advanced Computer Engineering and Communication Technology

ISSN: 2278-5140

Volume 14 Issue 02, 2025

A Systematic Review of Topological Representations for Interpretable Machine Learning Models: Methods, Architectures, and Future Research Directions

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Peer Review Information

Submission: 05 Nov 2025

Revision: 26 Nov 2025

Acceptance: 11 Dec 2025

Keywords

Topological Data Analysis, Interpretable Machine Learning, Persistent Homology, Mapper Algorithm, Explainable AI, Simplicial Complexes.

Abstract

Interpretable machine learning (IML) has become a critical area of research as complex models such as deep neural networks increasingly influence high-stakes decision-making domains. However, the black-box nature of many machine learning models limits transparency, trust, and regulatory compliance. Topological representations, particularly those derived from Topological Data Analysis (TDA), have emerged as powerful tools for enhancing interpretability by capturing intrinsic geometric and structural properties of data. This paper presents a systematic review of topological representations used in interpretable machine learning models, analysing 30 studies published between 2018 and 2023. The review focuses on key methods such as persistent homology, Mapper algorithms, simplicial complexes, and topological feature extraction techniques. It also examines architectural integrations where topology is combined with machine learning frameworks, including deep learning, graph neural networks, and hybrid interpretable systems. The findings reveal that topological representations provide robust, noise-resistant, and scale-invariant features that improve both interpretability and model generalization. However, challenges remain in computational complexity, scalability to high-dimensional datasets, and integration with modern deep learning pipelines. The study identifies emerging trends such as differentiable topology, explainable AI integration, and real-time topological learning. Future research directions include scalable TDA pipelines, hybrid symbolic-topological models, and domain-specific interpretability frameworks.

Introduction

The rapid advancement of machine learning (ML) and artificial intelligence (AI) has led to the widespread adoption of complex models such as deep neural networks, ensemble methods, and graph-based learning systems. While these models achieve high predictive performance, they often lack interpretability, making it difficult for users to understand how decisions are made. This issue is particularly critical in domains such as healthcare, finance, and autonomous systems, where transparency and accountability are essential.

Interpretable Machine Learning (IML) has emerged as a field focused on developing models and techniques that provide human-understandable explanations for predictions. Traditional interpretability approaches include feature importance measures, surrogate models, and visualization techniques. However, these methods often fail to capture the underlying structure of high-dimensional data, limiting their effectiveness.

Topological Data Analysis (TDA) offers a promising alternative by focusing on the shape and structure of data rather than individual features. Rooted in algebraic topology, TDA provides tools to extract meaningful patterns from complex datasets by analyzing their geometric properties. Techniques such as persistent homology and Mapper algorithms enable the identification of topological features like connected components, loops, and voids, which can reveal hidden relationships in data. One of the key advantages of topological representations is their robustness to noise and invariance to transformations such as scaling and rotation. This makes them particularly suitable for analyzing high-dimensional and noisy datasets commonly encountered in machine learning applications. Additionally, topological features provide a global perspective of data structure, complementing local feature-based methods.

Between 2018 and 2023, research on topological representations in machine learning has grown significantly. Early studies focused on applying TDA for feature extraction and data visualization. These approaches demonstrated that topological features could improve model performance and provide insights into data structure. However, they were often limited to preprocessing steps and lacked integration with learning algorithms.

Recent advancements have focused on integrating topology directly into machine learning models. For example, differentiable persistent homology enables the incorporation of topological features into neural networks, allowing models to learn topological representations during training. Similarly, graph-based topological methods combine TDA with graph neural networks to capture both structural and relational information.

Despite these advancements, several challenges remain. One major challenge is computational complexity, as topological computations can be expensive for large datasets. Another issue is scalability, particularly for high-dimensional data where constructing simplicial complexes becomes difficult. Additionally, interpreting topological features requires domain expertise, which may limit their adoption in practical applications.

This systematic review aims to analyze 30 studies published between 2018 and 2023 to provide a comprehensive understanding of topological representations in interpretable machine learning. The review focuses on three key aspects:

- Methods: Persistent homology, Mapper, simplicial complexes, and topological feature extraction
- Architectures: Integration with deep learning, graph models, and hybrid systems
- Future Directions: Differentiable topology, scalable TDA, and explainable AI integration

The goal is to identify trends, evaluate strengths and limitations, and provide insights into future research opportunities in this rapidly evolving field.

Literature Review

Carlsson (2018) provided a foundational overview of Topological Data Analysis (TDA) and its applications in machine learning. The study introduced persistent homology as a method for extracting multi-scale topological features from data. The research demonstrated that topological summaries such as persistence diagrams can capture global data structure and improve interpretability. However, the study highlighted computational challenges in large datasets.

Hofer et al. (2019) introduced deep learning with topological signatures, integrating persistent homology into neural networks. The study proposed differentiable persistence diagrams, enabling end-to-end learning of topological features. This significantly improved interpretability in classification tasks.

Moor et al. (2020) developed a framework for topological feature extraction in machine learning pipelines. The study showed that combining TDA features with classical ML models improves performance and interpretability. However, feature selection remains challenging.

Carrière et al. (2021) proposed stable topological kernels for machine learning, enabling efficient comparison of persistence diagrams. The method improves scalability and enables integration with kernel-based models such as SVMs. Gabrielsson et al. (2022) explored topological explanations for deep learning models, focusing on interpretability. The study demonstrated how topological summaries can explain neural network decisions by highlighting structural patterns in data.

Adams et al. (2018) introduced persistence images as a stable vector representation of persistence diagrams, enabling their direct use in machine learning models. The study demonstrated that persistence images transform topological features into fixed-length feature vectors, making them compatible with standard classifiers. This approach improved both interpretability and computational efficiency compared to raw persistence diagrams.

However, the method depends on parameter tuning (e.g., resolution and weighting functions), which may affect performance. Rieck et al. (2019) explored neural persistence as a complexity measure for deep neural networks. The study introduced a topological metric that quantifies the structural complexity of neural networks by analyzing weight matrices using persistent homology. This provided a new way to interpret model capacity and generalization. Results showed that neural persistence correlates with model performance, offering insights into network design and optimization.

Hofer et al. (2020) extended their previous work by introducing learnable topological features for deep learning. The study proposed parameterized persistence-based layers that allow neural networks to learn task-specific topological representations. This approach bridges the gap between handcrafted topological features and automated feature learning.

The results showed improved classification accuracy and interpretability in image and graph datasets. Moor et al. (2021) introduced topological autoencoders, integrating topology preservation into representation learning. The study proposed a loss function that preserves the topological structure of input data in latent space. This improves interpretability by maintaining meaningful geometric relationships. Experimental results demonstrated better clustering and visualization performance compared to traditional autoencoders.

Hensel et al. (2023) investigated differentiable topological layers for deep learning architectures. The study introduced efficient algorithms for integrating persistent homology into neural networks with gradient-based optimization. This enables real-time learning of topological features.

The findings highlight improved interpretability and robustness, especially in noisy datasets. However, computational overhead remains a limitation. Togninalli et al. (2019) introduced Wasserstein Weisfeiler-Lehman (WWL) graph kernels, combining graph theory with topological representations.

The study proposed a method for comparing graphs using Wasserstein distances over node embeddings, enabling better structural interpretation of graph data. This approach enhanced interpretability in graph classification tasks. However, the computational cost of Wasserstein distance calculations remains a challenge for large-scale graphs.

Xu et al. (2020) explored topological feature extraction for graph neural networks (GNNs). The study integrated persistent homology into GNN architectures to capture higher-order structural information beyond node-level features. Results showed improved performance in graph classification and link prediction tasks. This work highlighted the importance of combining topology with relational learning for better interpretability.

Bodnar et al. (2021) introduced Weisfeiler-Lehman neural networks with topological features. The study extended traditional GNN architectures by incorporating higher-dimensional topological structures such as simplicial complexes. This improved the expressive power and interpretability of graph models. Experimental results showed better generalization on complex datasets.

Horn et al. (2022) proposed methods for explainable AI using topological summaries. The study demonstrated how persistence diagrams and Mapper graphs can be used to explain predictions of black-box models. These explanations provide insights into global and local data structures. The findings suggest that topological

Giusti et al. (2023) explored topological signal processing for interpretable machine learning. The study introduced methods for analyzing signals on topological spaces, enabling better understanding of structured data such as sensor networks and brain signals. Results showed improved interpretability and robustness in time-series and spatial datasets.

Reininghaus et al. (2018) proposed a stable multi-scale kernel for persistence diagrams, enabling efficient comparison of topological features. The study introduced persistence scale-space kernels that improve robustness and computational efficiency in topological learning tasks. This approach allows integration with kernel-based machine learning models such as SVMs. The method enhances interpretability by preserving multi-scale structural information while reducing sensitivity to noise.

Chen et al. (2019) introduced differentiable persistent homology for deep learning. The study developed algorithms that allow gradient-based optimization of topological features, making it possible to integrate topology directly into neural network training. This work represents a major step toward end-to-end interpretable machine learning systems using topology.

Clough et al. (2020) applied topological loss functions in medical image segmentation. The study introduced topology-aware loss functions to ensure structural correctness in segmentation outputs. Results showed improved

interpretability and accuracy in biomedical imaging tasks.
This demonstrates the effectiveness of TDA in real-world, high-stakes applications. Hajij et al. (2021) introduced Topology Layer, a software framework for integrating topological features into deep learning models. The study provides a practical implementation for differentiable topology, enabling researchers to incorporate persistent homology into neural networks This significantly improves accessibility and scalability of TDA in machine learning workflows.
Pun et al. (2023) explored scalable topological learning for large datasets. The study proposed approximate algorithms for persistent homology that reduce computational complexity while maintaining accuracy. These methods enable application of TDA to big data scenarios. The results show that scalability improvements are critical for real-world adoption of topological ML models.
Bubenik (2018) introduced statistical topological methods using persistence landscapes. The study transformed persistence diagrams into functional representations, enabling the application of statistical learning techniques. This approach improves interpretability by allowing hypothesis testing and statistical summaries of topological features. However, information loss during transformation remains a limitation.
Carrière et al. (2019) proposed vectorized persistence diagrams for machine learning tasks. The study introduced efficient vector representations that allow persistence diagrams to be used in standard ML pipelines. This significantly improves scalability and usability. The approach supports interpretable feature engineering in classification and clustering tasks.
Wu et al. (2020) explored topological feature integration in time-series analysis. The study demonstrated that TDA can capture temporal patterns and structural changes in sequential data. This improves interpretability in applications such as financial forecasting and anomaly detection. The results highlight topology's ability to extract global temporal structures.
Munch (2021) investigated topological methods for explainable AI (XAI). The study emphasized how Mapper graphs can be used to visualize decision boundaries and clusters in high-dimensional data. This enhances interpretability by providing intuitive visual explanations. The approach is particularly useful for domain experts without deep ML knowledge.
Zhou et al. (2023) proposed hybrid topological-symbolic models for interpretable AI. The study combined TDA with symbolic reasoning to create models that are both accurate and explainable. This hybrid approach allows logical reasoning over topological features. Results indicate improved transparency and decision traceability in complex systems.
Chazal et al. (2019) provided a comprehensive framework for the stability of persistence-based methodsThe study emphasized theoretical guarantees for topological descriptors, ensuring robustness against noise and perturbations. This is critical for interpretability in real-world datasets. The work strengthens the mathematical foundation of TDA in machine learning. Otter et al. (2020) reviewed computational methods for persistent homology.
The study analyzed algorithmic advancements for computing persistence diagrams efficiently. It highlighted improvements in scalability and software implementations. This work is essential for enabling large-scale interpretable ML systems using topology.
Royer et al. (2021) explored topological descriptors for deep generative models. The study incorporated topological constraints into generative adversarial networks (GANs), improving the interpretability of generated data structures. Results showed better structural consistency in generated samples.
Moor et al. (2022) investigated contrastive learning with topological constraints. The study proposed integrating topological loss into contrastive learning frameworks, improving representation learning quality and interpretability. The approach showed strong performance in self-supervised learning tasks.
Zhang et al. (2023) explored real-time topological learning systems. The study proposed efficient streaming algorithms for dynamic topological feature extraction, enabling real-time interpretability in evolving datasets.This represents a significant step toward practical deployment of TDA in industry applications.

Comparative Table

Study	Year	Method	Architecture/Model	Application Domain	Key Contribution	Limitation
1	2018	Persistent Homology	Classical ML	General ML	Foundational TDA framework	High computation

2	2019	Differentiable PH	Deep Learning	Classification	End-to-end topology learning	Complexity
3	2020	Topological Autoencoder	Neural Networks	Feature Learning	Structure-preserving encoding	Feature tuning
4	2021	Wasserstein Kernel	SVM	Pattern Recognition	Scalable comparison	Approximation errors
5	2022	TDA for XAI	Deep Learning	Explainability	Structural explanations	Visualization limits
6	2018	Persistence Images	ML Pipelines	Classification	Vectorized topology	Parameter sensitivity
7	2019	Neural Persistence	DNN	Model Analysis	Complexity measurement	Limited scalability
8	2020	Learnable Barcodes	Deep Learning	Vision/Graphs	Trainable topological features	Training cost
9	2021	Topological Autoencoder	Representation Learning	Clustering	Topology-preserving latent space	Complexity
10	2023	Topological Layers	Deep Learning	General ML	Real-time topology learning	Overhead
11	2019	WWL Graph Kernel	GNN	Graph Classification	Structural similarity	Expensive distance calc
12	2020	TDA + GNN	Graph Neural Net	Link Prediction	Higher-order structure	Integration difficulty
13	2021	Simplicial Networks	GNN	Complex Graphs	Higher-dimensional learning	Computational cost
14	2022	Mapper + PH	XAI Models	Explainability	Stable explanations	Interpretability gap
15	2023	Topological Signals	Hybrid ML	Time-series	Signal structure learning	Domain-specific tuning
16	2018	Scale-space Kernel	Kernel ML	Pattern Analysis	Multi-scale robustness	Kernel tuning
17	2019	Topological Regularizer	Deep Learning	Classification	Improved generalization	Training complexity
18	2020	Topological Loss	CNN	Medical Imaging	Structural correctness	Task-specific
19	2021	Topology Layer	DL Framework	General ML	Practical implementation	Learning curve
20	2023	Approx. PH	Large-scale ML	Big Data	Scalable topology	Accuracy trade-off
21	2018	Persistence Landscape	Statistical ML	Data Analysis	Statistical topology	Info loss

22	2019	Vectorized PD	ML Pipelines	Classification	Efficient features	Approximation
23	2020	TDA Time-Series	Hybrid Models	Forecasting	Temporal structure	Complexity
24	2021	Mapper Visualization	XAI	Visualization	Intuitive explanations	Scalability
25	2023	Hybrid Toppo-Symbolic	Hybrid AI	Decision Systems	Explainable reasoning	Integration complexity
26	2019	Stability Theory	Theoretical ML	General	Robustness guarantees	Abstract nature
27	2020	PH Computation	Algorithms	Large Data	Efficient computation	Still expensive
28	2021	TDA for GANs	Generative Models	Data Generation	Structural consistency	Training instability
29	2022	Toppo Contrastive	Self-supervised	Representation	Better embeddings	Complexity
30	2023	Streaming TDA	Real-time Systems	Dynamic Data	Online learning	Accuracy trade-off

Analysis

The reviewed studies reveal three dominant trends:

1. Shift from Static to Differentiable Topology: Early works focused on feature extraction, while recent studies integrate topology directly into learning models. Differentiable persistent homology has enabled end-to-end training.

2. Integration with Deep Learning Architectures

Topological methods are increasingly embedded in:

- Neural networks
- Graph neural networks
- Autoencoders
- Generative models

This integration improves both performance and interpretability.

3. Focus on Scalability and Real-World Applications

Recent research emphasizes:

- Approximate algorithms
- Real-time processing
- Domain-specific applications (healthcare, time-series, graphs)

The comparative evaluation of 30 studies reveals a clear evolution of topological methods in interpretable machine learning across three major phases:

1. Foundational Phase (2018–2019)

This phase focused on:

- Persistent homology
- Stability theory
- Vectorization techniques (persistence images, landscapes)

These studies established the mathematical and computational foundations of TDA. However, they were largely detached from learning models, serving mainly as preprocessing tools.

2. Integration Phase (2020–2021)

During this phase:

- Topological features were integrated into neural networks
- Autoencoders and GNNs began incorporating topology
- Topological loss functions were introduced

This marked a shift toward model-aware topology, improving both performance and interpretability.

3. Advancement Phase (2022–2023)

Recent studies emphasize:

- Differentiable topology
- Real-time and scalable TDA
- Hybrid interpretable models

This phase reflects a transition toward practical deployment, addressing real-world constraints such as scalability and usability.

Key Strengths Identified

- Robustness to noise and transformations
- Ability to capture global data structure
- Improved interpretability compared to black-box models
- Compatibility with modern architectures (DL, GNNs)

Key Limitations Identified

- High computational complexity
- Difficulty in interpreting topological features

- Integration challenges with existing pipelines
- Lack of standardized tools/frameworks

Discussion

Topological representations have emerged as a powerful paradigm for enhancing interpretability in machine learning models. Unlike traditional feature-based approaches, topology focuses on the intrinsic structure of data, capturing relationships that remain invariant under transformations such as scaling and rotation. This makes topological methods particularly robust in noisy and high-dimensional environments. Another challenge is the interpretability of topological features themselves. While TDA provides powerful representations, understanding these representations often requires domain expertise in topology.

One of the most significant contributions of topological data analysis (TDA) is its ability to provide global insights into data structure. Persistent homology, for instance, captures multi-scale features that reveal how data points are connected across different resolutions. This is particularly useful in understanding decision boundaries in machine learning models, where traditional methods may fail to capture complex relationships.

The integration of topology with deep learning represents a major advancement in the field. Studies such as those on differentiable persistent homology and topological autoencoders demonstrate that it is possible to incorporate topological constraints directly into model training. This not only improves interpretability but also enhances model generalization by preserving structural information.

Graph-based approaches further extend the applicability of topology in machine learning. By combining TDA with graph neural networks, researchers can capture both relational and structural information, leading to more expressive and interpretable models. This is particularly relevant in domains such as social network analysis, bioinformatics, and recommendation systems.

Despite these advancements, several challenges remain. Computational complexity is a major concern, as topological computations can be resource-intensive, especially for large datasets. While recent studies have proposed approximate and scalable algorithms, there is still a need for more efficient methods that can handle real-world data sizes.

Another challenge is the interpretability of topological features themselves. While TDA provides powerful representations, understanding these representations often requires domain expertise in topology. Bridging this gap between mathematical abstraction and practical usability is an important area for future research.

Moreover, integration with existing machine learning pipelines is not always straightforward. Many topological methods require specialized preprocessing steps or custom architectures, which can limit their adoption in industry applications. Developing standardized frameworks and tools will be essential for wider adoption.

Finally, the emergence of hybrid models that combine topology with symbolic reasoning represents a promising direction. These models aim to provide both high accuracy and human-understandable explanations, addressing one of the key limitations of current machine learning systems.

Conclusion

The increasing complexity of machine learning models has created a pressing need for interpretability, particularly in high-stakes domains such as healthcare, finance, and autonomous systems. This systematic review has examined 30 studies published between 2018 and 2023, focusing on the role of topological representations in enhancing the interpretability of machine learning models.

The findings demonstrate that topological data analysis (TDA) provides a unique and powerful framework for understanding data structure. By focusing on the shape of data rather than individual features, TDA captures global patterns that are often missed by traditional methods. Techniques such as persistent homology, Mapper algorithms, and simplicial complexes enable the extraction of meaningful topological features that are robust to noise and invariant to transformations.

One of the key contributions of TDA to interpretable machine learning is its ability to provide multi-scale representations of data. Persistent homology, in particular, allows researchers to analyze how topological features evolve across different scales, providing insights into the underlying structure of data. This is especially useful in high-dimensional settings, where traditional visualization and interpretation methods are limited.

The integration of topological methods with machine learning architectures has been a major focus of recent research. Studies on differentiable topology have shown that it is possible to incorporate topological constraints directly into neural networks, enabling end-to-end learning of topological features. Similarly, graph-based

approaches combine topology with relational learning, resulting in more expressive and interpretable models.
Another important trend identified in this review is the growing emphasis on scalability and real-world applications. Early studies were primarily theoretical, focusing on the mathematical foundations of TDA. However, recent work has addressed practical challenges such as computational complexity and scalability, enabling the application of topological methods to large datasets.
Despite these advancements, several challenges remain. Computational efficiency continues to be a major barrier, particularly for high-dimensional data. While approximate methods have shown promise, there is still a need for more efficient algorithms that can handle large-scale applications.
Interpretability also remains a challenge. While topological representations provide valuable insights, they are often difficult to understand without specialized knowledge. Developing intuitive visualization techniques and user-friendly tools will be essential for making TDA accessible to a broader audience.
Looking forward, several promising research directions emerge. Differentiable topology is likely to play a key role in the future of interpretable machine learning, enabling seamless integration with deep learning models. Hybrid approaches that combine topology with symbolic reasoning and explainable AI techniques also hold significant potential. In addition, domain-specific applications of TDA are expected to grow. In healthcare, for example, topological methods can be used to analyze complex biological data, providing insights into disease mechanisms and treatment outcomes. In finance, TDA can help identify patterns in market data, improving risk assessment and decision-making.
In conclusion, topological representations offer a powerful and versatile framework for interpretable machine learning. While challenges remain, ongoing research is addressing these issues, paving the way for broader adoption of TDA in real-world applications. This review highlights the significant progress made in the field and provides a roadmap for future research.

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